DNAPL Infiltration in a Two-Dimensional Porous Medium–Influence of the Shape of the Solid Particles

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ABSTRACT *The infiltration with atmospheric pressure of Dense Non Aqueous Phase Liquid (DNAPL) in a model of porous media saturated by another liquid is studied when the DNAPL liquid has a contact angle characterizing wetting liquid. The model of porous media consists of an assembly of solid particles for various forms. The influence of the shape of the particles is studied.*

KEYWORDS: DNAPL; Multiphase flow; Wetting liquid; Solid particle; VOF

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The multiphase flows in the porous media are numerous in nature and various industrial processes. While being limited to the immiscible transport of pollutant with water known under the name of DNAPL (Dense Not Aqueous Liquid Phase), these flows meet in the geomaterials ones, the processes of remediation of the grounds, the biofilters employed in waste water treatment, etc… The properties of these flows are complex and often unknown because of a large number of physical parameters. At the present time, the influence of the density, the viscosity or the interfacial tension of DNAPL on its infiltration in the porous medium is studied much by several authors like Pennell and Al, 1996, Dawson and Roberts, 1997, Hofstee *et al.*, 2003, Jeong and Corapcioglu, 2005, Tartakovsky *et al.*,2007, Meakin *et al.*, 2009. Most of these studies are realized on a macroscopic scale which does not make it possible to understand the retention of small drops of DNAPL in the pores of the medium. However, few studies carried out at the level of the interstices showed the fractionation of the DNAPL as well in experiments as by numerical modeling (Krishna and van Baten 1999, Storr and Behnia 2000, Harvie *et al.*, 2006).

In this work, we highlight the influence of a parameter which is currently still less known - geometry of the solid particles of the porous medium - on the infiltration and the fractionation of a drop of DNAPL. Numerical modeling is carried out in two-dimensional configuration in order to decrease the computational time.

2. Problem Position

The fluids used in this study are water (carrier fluid) and the DNAPL (the drop). The density and the viscosity of water are of 998 kg.m^{-3} and 1.10^{-3} Pa.s. Those of the DNAPL are respectively equal to 1623 kg.m^{-3} and 0,89 Pa.s. As an example, Perchlorethylen (PCE) has these properties (INERIS, 2002). We imposed a contact angle of 65° in order to consider a wetting DNAPL because most of them being in nature are wetting.

Figure 1 presents one of the three structures of the porous medium used. This porous medium is represented by a regular assembly of similar and non deformable solid particles. The circle apart from the medium represents a drop of DNAPL at the initial time. It is injected without initial velocity within the carrying fluid which is at rest. Under the effect of the difference of the density between the carrying fluid and the drop, the latter infiltrates through the porous medium. The domain of calculation is rectangular. Its dimensions relative to the radius R of a solid particle are 12,5x18,1. It is composed of 3 zones. From top to bottom, zone1 contains the drop at t = 0, zone 2 contains the porous medium composed by 64 particles, zone 3 contains the wall of the bottom which is used to recover the infiltrated DNAPL.

The shape of a solid particle is described by the following equation which enables us to pass from the circular form to the almost square form by increasing the value of the parameter m :

$$\left(\frac{x}{R}\right)^{2m} + \left(\frac{y}{R}\right)^{2m} = 1$$

In this paper, we present three models of the porous medium which differ by the form of the solid particles by varying m: m = 1 (circle), m = 2 and m → ∞ (square). In view to conserve the same porosity (0.36), we vary the side a of the square mesh (see figure 2) while preserving R constant.

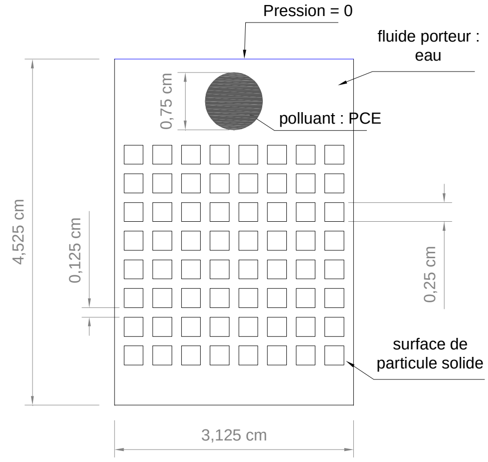

Figure 1 Description of the computational domain, case $m \to \infty$

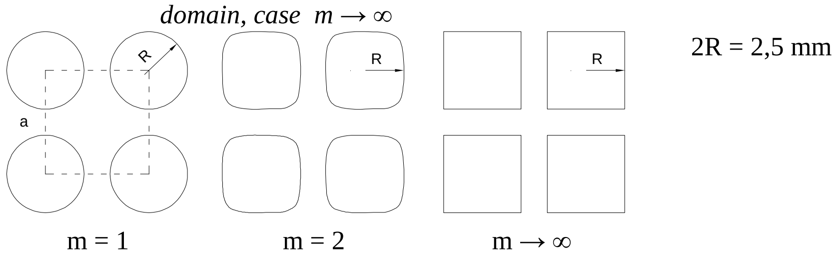

Figure 2 Shape of the solid particles

In this study, we use a numerical simulation based on algorithm VOF (Volume of Fluid). This algorithm is approached for the first time by Hirt and Nichols (1981). Besides solving the Navier-Stokes equation, these two authors introduced the definition of the volume fraction χ of two immiscible fluids (1 and 2) into the mesh. The volume fraction is equal to 0 in fluid 1, equal to 1 in fluid 2 or between 0 and 1 within the interface of the fluids. Here fluid 1 is the main fluid. The volume fraction with the interface is controlled by the equation:

$$\frac{\partial \chi}{\partial t} + \vec{u}.\vec{\nabla}\chi = 0$$

The surface tension model, known as continuum surface force (CSF) model, proposed by Brackbill *et al.* (1992) is used to track the interface.

3. Results and discussion

Figure 3 shows the infiltration of a drop in each of the models presented in figure 2. The results are presented in function of time. For generalization, time can ce normalized by the time of settling of the drop in an infinite static continuous flow field. The settling velocity found by Hadamard, 1911; Rybczynski, 1911 for small Reynolds number is

$$U_{d\infty} = \frac{gd^2\Delta\rho}{2\mu_c}\frac{(1+\lambda)}{(6+9\lambda)}$$

Where $\Delta\rho$ is the difference of densities, λ is the ratio of the drop viscosity and the continuous fluid viscosity, μ_c is the viscosity of the continuous fluid. For water as continuous fluid and PCE as the drop, the value of the settling velocity is 31.7 $mm.s^{-1}$ and the reference time is thus $t_0=d/U_{d\infty}=0.24s$.

We observe that for the three models of the porous medium studied, the drop is spread out initially horizontally and then infiltrates vertically. The drop tries to maintain its volume constant but the more deeply it infiltrates, the more it is divided into several droplets. By comparing the infiltration in these three models, we note that when m increases, separation of the principal drop onto droplets is important.

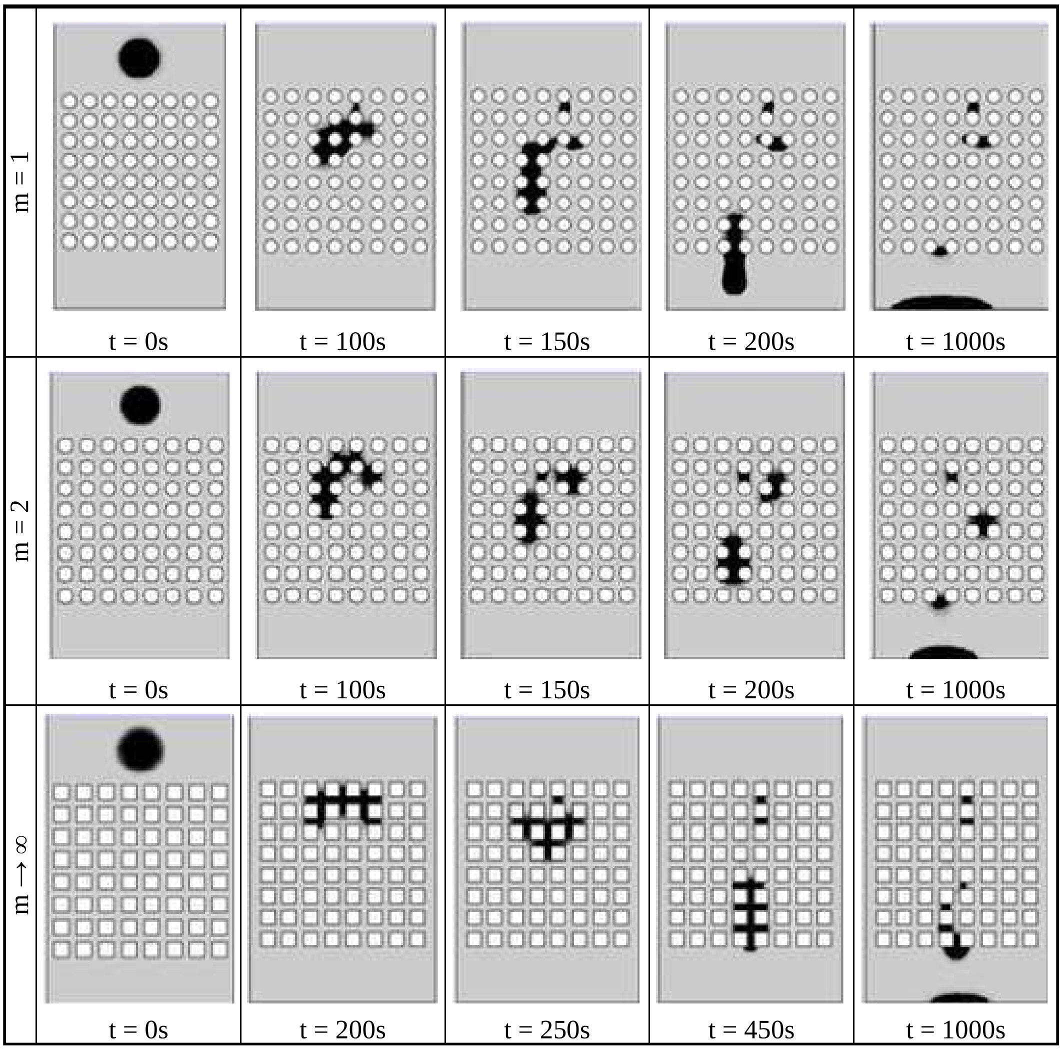

Figure 3 Behavior of a DNAPL drop during infiltration in a model of porous medium

The droplets resulting from the fractionation of the principal drop are retained in these porous medium either between two solid particles rows vertically, or between two solid particles rows horizontally, or between four solid particles.

Figure 4 explains the mechanism of retention of the droplets in contact with two solid particles of an horizontal row.

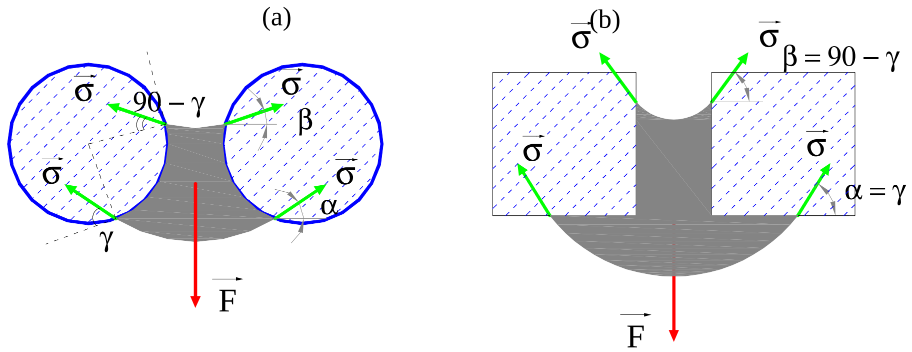

Figure 4 Illustration of the mechanism of drop retention

$\vec{\sigma}$ represents the contact force ;

$\vec{F}$ represents the apparent weight of the drop

We note that surface of the liquid/solid contact increases with increasing the parameter m. This surface is minimum for the case where the solid particles are circles. The more surface of the liquid/solid contact increases, the more adherence on the area of this contact increases. That explains why for the cases m > 1, the drops are retained between the solid particles with increasingly large volume as m increases.

We compare then the velocity of the infiltration of the DNAPL in the different models of the porous medium. For each model, calculation is carried out until the moment when the immobility of the drop becomes permanent. We present in figure 5a the depth of the infiltration (vertical position of the lower face of the drop relatively to the surface of the porous medium) according to time for the three models. We find that the velocity of the infiltration of DNAPL decreases when m increases. Figure 5b shows the volume of retention of DNAPL in the different models of the porous medium. The parameter V_r/V_t defines the ratio of the volume of DNAPL retained in the medium on the total volume of DNAPL injected. In the case of the particles having the circular form, most of the drop passes through the porous medium. There is only 30% of the volume of the drop which is retained in the pores. When the shape of the particles tends towards the square form, the volume of DNAPL retained in the pores increases. It reaches 64% and 72% respectively for the case m = 2 and the case of the square.

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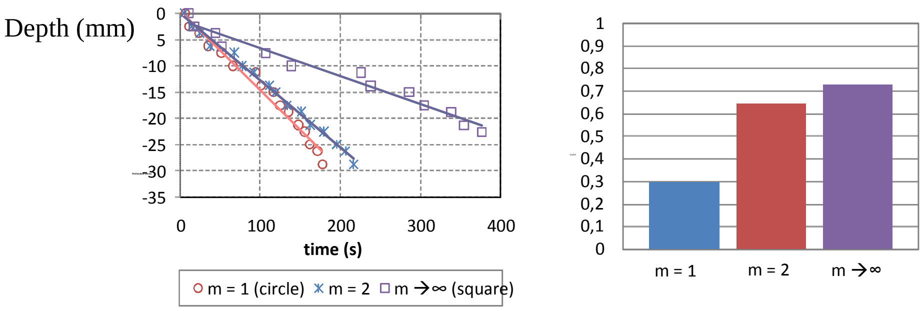

(a) (b)

Figure 5

(a) DNAPL infiltration velocity ;

(b) DNAPL retention volume

4. Conclusion

The analysis of the influence of the shape of the solid particles on the infiltration of the DNAPL is carried out for several forms: circular, square, intermediate form enter the circle and the square. This study highlights that as the shape of the particles passes from the circle shape to the square shape, the speed of infiltration decreases while the retention of the DNAPL increases. This retention is the result of the fractionation of the drop.

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